GAS CHROMATOGRAPHY AND MASS SPECTROMETRY MEASUREMENTS AND PROTOCOLS FOR DATABASE AND LIBRARY DEVELOPMENT RELATING TO ORGANIC SPECIES IN SUPPORT OF THE MARS SCIENCE LABORATORY.

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This paper describes the development of an organic contaminants database for the Sample Analysis at Mars (SAM) instrumentation suite in support of the Mars Science Laboratory (MSL) mission in 2011 by utilizing Gas Chromatography-Mass Spectrometry (GC-MS) analysis tools. It will allow us to determine which compounds are found here on Earth and would be inadvertently detected in the Mars soil and gaseous samples as impurities. In order to develop a comprehensive target database, we utilize the National Institute of Standards & Technology (NIST) Automated Mass Spectral Deconvolution and Identification System (AMDIS) and Ion Signature Technology's Ion Fingerprint Deconvolution (IFD) software to laboratory-based GC-MS rover data. We use the compound spectra added to the library to identify compounds that might be found as impurities from potential mission samples.

Contamination due to outgassing of spacecraft materials is a significant issue for *in situ* organic analysis on planetary surfaces. Several studies have been done on outgassing of polymeric materials, e.g. Young and Slemp (1998), Rampini et al. (2003), Chang (2004), and Villahermosa and Joseph (2004). Contamination control is critical for several areas of terrestrial geochemical research, and lessons learned from ocean floor research and glacial ice cores, for example, can be useful for space mission planning (Christner et al., 2003; Grosjean and Logan, 2007; Eigenbrode et al., 2009). To address this contamination problem, NASA commissioned an Organic Contamination Science Steering Group (OCSSG), which identified the primary areas of focus prior to the announcement of opportunity for the MSL Mission. These strategies were developed to provide direction for the engineering and operations teams responsible for the design, fabrication, assembly, and operations of Mars landed systems and the science teams responsible for analysis of the data from Mars (Mahaffy et al., 2003). Some of these strategies were also employed during the Viking mission (Flory et al., 1974).

Database files are currently in excel spreadsheet format, and once we obtain all the pertinent information from the files, we plan to develop a more interactive and user-friendly database that will be searchable through an interface rather than having to access it directly from files. We add spectra to a library in MSP format and edit the parameter information based on what the NIST library search determines (i.e., identify the unknown compound, name it and give it the corresponding compound element composition). Once done, we import it into the NIST MS Search program and create a NIST-formatted library from the exported spectra.

The file database is a spreadsheet file that contains file locations with information on the runtime parameters and the environment in which the tests were conducted. The purpose of this database is to keep track of the conditions under which each file was recorded, so that we are able to better assess its similarity when comparing it with data taken in the Mars environment. The contaminants database is a reference spreadsheet file that contains the compounds found in each file and how they can be identified by their library names. Its primary purpose is to identify each compound that has been found in each of the files that corresponds to a material sample.

The data we are currently analyzing are GC-MS files that have been run on a Finnigan SSQ7000 Thermal Desorption Model 2000 Gas Chromatograph using a SGE Forte GC Capillary Column HT5 of length: 25m, I.D: 0.22mm and Film: 0.1µm. The data contains information about possible compounds in the rover material samples that have been supplied by JPL and have been pyrolized. Materials such as polymers, paint, o-rings are some examples of the material samples that are pyrolized in this process.

The results from the analysis done on the Hysol EA9360 GCMS are presented here in Table 1 and summarize the TIC Peak identification using the Ion Fingerprint Deconvolution (IFD) software. As can be seen from the table, some of the spectra obtained from these files have very high match/rmatch ratios and probabilities. Some of the cells exhibit a very high match - to the point that we can say that the unknown spectrum and the spectrum NIST matches it with are nearly identical - as illustrated in Fig. 1. Other cells indicate a good match, but with a higher amount of peak differences. In both cases, however, the matched spectrum retains the general shape of the unknown spectrum.

Table 1. GC-MS Analysis of Hysol EA9360 Sample

Ret.Time [min.]	Chemical Name	Match	Prob
7.02	Phenol	0.996845	7130
7.6	4-Cyanocyclohexene	0.994505	4654
8.03	Benzyl Alcohol	1	7849
11.17	5-Amino-1,3,3-trimethylcyclohexanemethylamine	1	8783
11.33	5-Amino-1,3,3-trimethylcyclohexanemethylamine	1	9684
12.411	1-Dodecanol	0.995708	2425
15.36	Phenanthrene-D10	0.998921	7627
16.048	Hexadecanoic acid, methyl ester	0.996703	7266
17.29	9-Octadecenoic acid, methyl ester, (E)-	0.990142	1952
17.41	Octadecanoic acid, methyl ester	0.996746	6365
17.792	Hexadecanoic acid, butyl ester	0.964871	6455
19.185	O-Benzyl-L-tyrosine	0.961436	2425
19.415	2,2'-Ethylidenebis(4,6-di-tert-butylphenol)	0.969061	9570
20.172	Eicosanoic acid, phenylmethyl ester	0.887425	8098
22.62	Oxirane, 2,2'-[(1-methylethylidene)bis(4,1-phenyleneoxymethylene)]bis-	1	9818
24.77	Chromone, 2-[2-[3,5-dihydroxyphenyl]ethenyl]-5-hydroxy-	0.927536	5320
43.22	2-Phenyl-4,6-di(4-acetylaminophenyl)pyrimidine	0.85025	2312

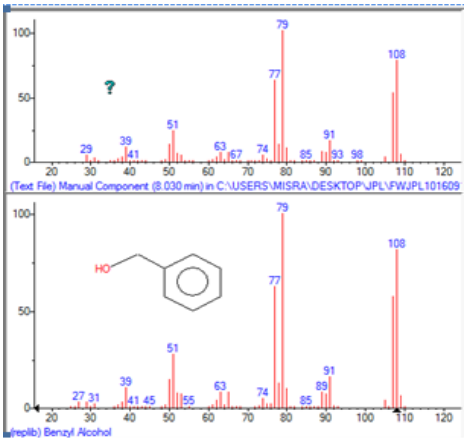

Fig. 1. Illustration of good library spectral match.

Fig. 2 illustrates a poor match, since the most likely compound identified by NIST does not share similar properties with the sample. Based on such analyses, we have been able to identify the compounds that are found in our data and are continually adding them to expand the contaminants database.

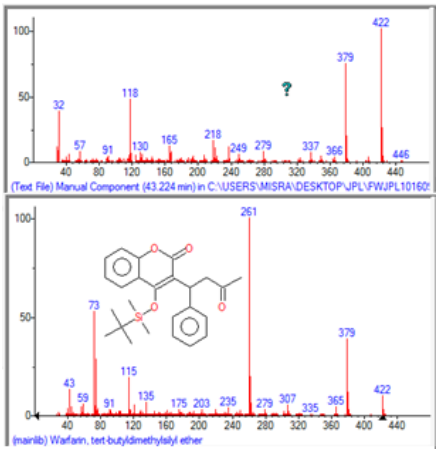

Fig. 2. Illustration of poor library spectral match.

We have successfully developed an initial target compound database that will aid SAM in determining whether the components being analyzed come from Mars or are contaminants from either the rover itself or the Earth environment. Future development will be geared towards gaining access to the information contained in these database spreadsheets via a command prompt file search routine.

References:

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